Journal of Hydrology 523 (2015) 725–738

Contents lists available at ScienceDirect

Journal of Hydrology

journal homepage: www.elsevier.com/locate/jhydrol

Does textural heterogeneity matter? Quantifying transformation of hydrological signals in soils

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ARTICLE INFO

Article history:
Received 4 November 2014
Received in revised form 30 January 2015
Accepted 4 February 2015
Available online 12 February 2015
The manuscript was handled by Corrado Corradini, Editor-in-Chief, with the assistance of Christophe Darnault, Associate Editor

Keywords:
Soil heterogeneity
Soil moisture time series
Principal component analysis
Transformation of hydrological signals
Functional averaging
Numerical experiment

SUMMARY

Textural heterogeneity causes complex water flow patterns and soil moisture dynamics in soils that hamper monitoring and modeling soil hydrological processes. These patterns can be generated by process based models considering soil texture heterogeneities. However, there is urgent need for tools for the inverse approach, that is, to analyze observed dynamics in a quantitative way independent from any model approach in order to identify effects of soil texture heterogeneity. Here, studying the transformation of hydrological input signals (e.g., rainfall, snow melt) propagating through the vadose zone is a promising supplement to the common perspective of mass flux considerations. In this study we applied a recently developed new approach for quantitative analysis of hydrological time series (i) to investigate the effect of soil texture on the signal transformation behavior and (ii) to analyze to what degree soil moisture dynamics from a heterogeneous profile can be reproduced by a corresponding homogenous substrate. We used simulation models to generate three data sets of soil moisture time series considering homogeneous substrates (HOM), homogeneous substrates with noise added (NOISE), and heterogeneous substrates (HET). The soil texture classes sand, loamy sand, clay loam and silt were considered. We applied a principal component analysis (also called empirical orthogonal functions) to identify predominant functional patterns and to measure the degree of signal transformation of single time series. For the HOM case 86.7% of the soil moisture dynamics were reproduced by the first two principal components. Based on these results a quantitative measure for the degree of transformation of the input signal was derived. The general nature of signal transformation was nearly identical in all textures, but the intensity of signal damping per depth interval decreased from fine to coarse textures. The same functional patterns occurred in the HET data set. However, here the signal damping of time series did not increase monotonically with soil depth. The analysis succeeded in extracting the same signal transformation behavior from the NOISE data set compared to that of the HOM case in spite of being blurred by random noise. Thus, principal component analysis proved to be a very robust tool to disentangle between independent effects and to measure the degree of transformation of the input signal. The suggested approach can be used for (i) data processing, including subtracting measurement noise (ii) identification of factors controlling soil water dynamics, (iii) assessing the mean signal transformation in heterogeneous soils based on observed soil moisture time series, and (iv) model building, calibration and evaluation.

1. Introduction

Textural heterogeneity of soils is a widespread phenomenon occurring at almost every location of the subsurface (Schulz et al., 2006). An important consequence is that water fluxes in the vadose zone occur in heterogeneous flow fields. This substantially complicates predicting subsurface fluxes by simulation models. No generally accepted model approach to easily simulate heterogeneous flow fields recently exist (cf. Vereecken et al., 2007). Inherent non-linearities of soil hydrological processes complicate modeling of soil water dynamics. Consequently, spatially aggregating of soil structural properties usually yields different model results than considering explicit small scale soil structure heterogeneities. However, considering such heterogeneities in high spatial resolution is feasible only at very small scales and with great effort. Hence, it is necessary to investigate inherent

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http://dx.doi.org/10.1016/j.jhydrol.2015.02.009
0022-1694/

characteristics of soil moisture time series from heterogeneous flow fields in order to find new efficient ways to consider textural heterogeneity in simulation models.

Effects of soil structure heterogeneity on soil water flow fields has often been studied by physically based models, i.e., generating time series of soil hydrological behavior (e.g. soil water flux q [$L\,T^{-1}$] or soil moisture θ [$L^3\,L^{-3}$]) as a function of soil structure and input fluxes (Köhne et al., 2009; Vereecken et al., 2007). However, the reverse approach, i.e., assessing effects of soil structure heterogeneities based on analysis of observed behavior is hardly feasible due to possible equifinality. Moreover, this approach has scarcely been investigated before. Overcoming this obstacle would allow to determine (i) to what degree properties of soil structure impose characteristic patterns on observed behavior, (ii) to what degree any observed behavior of heterogeneous soils could be modeled using a corresponding homogeneous substrate, and (iii) how the latter could be identified based on observed soil hydrological behavior.

In soil hydrology, soil water dynamics are usually regarded from the aspect of mass fluxes that can be modeled with flow and transport equations (van Genuchten et al., 2014). Here we suggest focusing on the aspect of transformation of a hydrological input signal (e.g., rainfall, snow melt) as it propagates through the soil. We define hydrological signals as spatiotemporal changes of state variables (e.g. pressure head, water level) that are propagated through a sequence of hydrological subsystems (e.g. aquifers or streams). In the vadose zone hydrological signals are processed by a change of soil moisture over time and space. In a homogeneous soil, an input signal becomes increasingly smoothed (Pan et al., 2011) and delayed (Mahmood et al., 2012) with soil depth.

In contrast, soil moisture dynamics emerging from heterogeneous flow fields are not only determined by soil depth and texture. They are also controlled by the usually randomly chosen position in a network of flow channels surrounded by regions with less mobile water (Schelle et al., 2013). Heterogeneous flow fields or non-uniform water fluxes can occur under various conditions. The most prominent reasons for such preferential flow patterns are macropore flow (Jarvis, 2007; Köhne et al., 2009), finger flow induced by water repellency (Diamantopoulos et al., 2013; Hendrickx et al., 1993; Ritsema and Dekker, 2000), and textural heterogeneity. The latter was investigated by Kung (1990a,b) who described distinct water pathways emerging from flow concentration at the top of inclined sand layers underlying finer textured substrates. This phenomenon called funneled flow was related to the occurrence of capillary barriers. It was intensively studied in the field (Heilig et al., 2003), in the laboratory (Kung, 1993; Walter et al., 2000) and by means of numerical experiments (Schlüter et al., 2012b). Roth (1995) performed numerical simulations of steady state flow through a Miller-similar medium (Miller and Miller, 1956). He showed that local heterogeneities of soil hydraulic properties in macroscopic homogeneous substrates can also evoke complex networks of flow channels. This approach was frequently used to represent heterogeneous flow fields in numerical models (e.g. Hohenbrink and Lischeid, 2014; Peters and Durner, 2009; Vogel et al., 2010).

Soil moisture dynamics at a specific location depend on the interplay of preceding local fluxes. An interesting question is whether non-linear interaction of preceding fluxes causes dynamics of soil moisture that could not occur in a homogeneous flow field. This would mean that non-linearity increases the complexity of soil moisture patterns. This question is of particular importance for upscaling purposes:

- If this would be the case, seepage fluxes at investigation sites could only be predicted on the basis of detailed information about spatial soil texture distributions. In the last decades great efforts have been made to map soil structures by non-invasive geophysical methods (e.g. Haarder et al., 2011; Koszinski et al., 2013). Resulting structural information has been included to inverse soil hydrological modeling (e.g. Busch et al., 2013; Hinnell et al., 2010; Kowalsky et al., 2004). Vogel et al. (2006) performed a dye tracer experiment in a structured soil and reconstructed geometry of observed structural components in a three dimensional model domain. They considered soil horizons, mesoscopic heterogeneity and macropores. Afterwards, they simulated water flow and tracer transport using the Richards Equation. Such analyses require much effort that can only be done in single studies at very small spatial scales.
- If this would not be the case, it would be rather possible to replace heterogeneous profiles in models by homogeneous surrogates (e.g. Greco et al., 2013) paving the way for upscaling approaches. Soil profiles showing similar response to input events (similar functional properties) could be aggregated to functional units (Lin et al., 2006). A large number of scientific papers deals with finding effective soil hydraulic properties (e.g. Bayer et al., 2005; Durner et al., 2008) and averaging vadose zone variables (e.g. De Lannoy et al., 2007; Schlüter et al., 2012a; Vogel et al., 2010). Most of these studies aimed at modeling heterogeneous soil water fluxes effectively with the one-dimensional Richards Equation.

Several authors stressed a common need for robust tools to identify and predict spatiotemporal patterns in soil science and hydrology (Grayson et al., 2002; Lin et al., 2006; Schröder, 2006). This includes functional patterns i.e. principal characteristics of system behavior that can be identified by intrinsic properties of measured time series. A promising way to evaluate functional patterns is to investigate how hydrological input signals propagate through a soil profile. It might be expected that the signal transformation behavior is a function of various processes related to soil properties, their heterogeneities, and soil depth. Transformation of soil moisture signals was more often studied in a meteorological context of atmosphere/subsurface interactions (Mahmood et al., 2012; Oudin et al., 2004; Wu et al., 2002) than with respect to soil hydrological questions like deep seepage (Wu et al., 1997). Lischeid et al. (2010) used a principal component analysis (PCA) to identify basic patterns of water signal transformation in unconfined aquifers and to quantify the intensity of signal damping in measured time series.

The aim of this study was to (i) investigate the effect of soil texture on the signal transformation behavior of homogeneous profiles and to (ii) analyze to what degree soil moisture dynamics simulated at any location of a heterogeneous profile can be reproduced by a corresponding homogenous substrate. For this purpose we performed numerical experiments to investigate and compare transformation characteristics of hydrological signals propagating homogeneous and heterogeneous profiles. In addition, we studied the effect of measurement errors trying to distinguish these effects from those of soil structure heterogeneities. We only considered flow processes occurring in the soil matrix that can conceptually be modeled by the Richards Equation. This includes uniform flow, finger flow, funneled flow and flow affected by local heterogeneities. Our intention was to investigate signal damping characteristics emerging from purely gravity driven flow without considering effects like root water uptake, capillary rise from groundwater or evaporation. We followed the approach that has recently be introduced by Lischeid et al. (2010). Thus, we used time series simulated for simple model scenarios instead of complex monitoring data in order to avoid confusion introduced by uncertain variables like evapotranspiration. In this paper we used the term functional heterogeneity to describe the variability in signal transformation behavior of soil profiles. Functional heterogeneity